lmalg

This subroutine has the interface for calling the function *lmder* from MINPACK. *lmder* is a modified levenberg-marquardt algorithm with analytically calculated jacobian.

[called by: solvers.] [calls: packdof.]

General

Levenberg-Marquardt algorithm is one of the most famous minimization algorithms. There is a brief introduction on Wikipedia. In FOCUS, we use the subroutine *lmder* from MINPACK.

Documentation

The cost functions (targets) are stored in **LM_fvec(1:LM_mfvec)**, and the jacobian is stored in **LM_fjac(1:LM_mfvec, 1:Ndof)**. The number of targets (**LM_mfvec**) must be not be smaller than the number of parameters (**Ndof**).

The targets are consistant of different terms. The following table lists the details. Here are the comments from *lmder*. The four

Table 1: **LM_fvec** components

cost functions	physiccal meaning	switch	length
bnormal	$\mathbf{B}\cdot\mathbf{n}$ on each surface element	weight_bnorm > 0	Nteta*Nzeta
bmnharm	$wBmn_i(Bmn_i - Bmn_i^o)$ for each reasonant harmonics	weight_bharm > 0	2*NBmn in *target.harmonics*
torflux	$\Psi_i - \Psi_o$ at each toroidal cross-sections	weight_tflux > 0	Nzeta
length	length penalty of each coil, $L_i - L_o$ or $\exp(L_i)/\exp L_o$	weight_ttlen > 0	Ncoils - Nfixgeo
surfsep	potential energy between each coil and a control surface	weight_cssep > 0	Ncoils - Nfixgeo

input parameters for L-M optimizer are LM_maxiter, LM_xtol, LM_ftol and LM_factor. Please look at initial for more details.

```
c     the subroutine statement is
c
c       subroutine lmder(fcn,m,n,x,fvec,fjac,ldfjac,ftol,xtol,gtol,
c                        maxfev,diag,mode,factor,nprint,info,nfev,
c                        njev,ipvt,qtf,wa1,wa2,wa3,wa4)
c
c     where
c
c       fcn is the name of the user supplied subroutine which
c         calculates the functions and the jacobian. fcn must
c         be declared in an external statement in the user
c         calling program, and should be written as follows.
c
c         subroutine fcn(m,n,x,fvec,fjac,ldfjac,iflag)
c         integer m,n,ldfjac,iflag
c         double precision x(n),fvec(m),fjac(ldfjac,n)
c
c         if iflag = 1 calculate the functions at x and
c         return this vector in fvec. do not alter fjac.
c         if iflag = 2 calculate the jacobian at x and
c         return this matrix in fjac. do not alter fvec.
c
c         return
c         end
c
c         the value of iflag should not be changed by fcn unless
c         the user wants to terminate execution of lmder.
c         in this case set iflag to a negative integer.
c
c       m is a positive integer input variable set to the number
c         of functions.
c
c       n is a positive integer input variable set to the number
c         of variables. n must not exceed m.
c
c       x is an array of length n. on input x must contain
c         an initial estimate of the solution vector. on output x
c         contains the final estimate of the solution vector.
c
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c       fvec is an output array of length m which contains
c         the functions evaluated at the output x.
c
c       fjac is an output m by n array. the upper n by n submatrix
c         of fjac contains an upper triangular matrix r with
c         diagonal elements of nonincreasing magnitude such that
c
c                t     t           t
c               p *(jac *jac)*p = r *r,
c
c         where p is a permutation matrix and jac is the final
c         calculated jacobian. column j of p is column ipvt(j)
c         (see below) of the identity matrix. the lower trapezoidal
c         part of fjac contains information generated during
c         the computation of r.
c
c       ldfjac is a positive integer input variable not less than m
c         which specifies the leading dimension of the array fjac.
c
c       ftol is a nonnegative input variable. termination
c         occurs when both the actual and predicted relative
c         reductions in the sum of squares are at most ftol.
c         therefore, ftol measures the relative error desired
c         in the sum of squares.
c
c       xtol is a nonnegative input variable. termination
c         occurs when the relative error between two consecutive
c         iterates is at most xtol. therefore, xtol measures the
c         relative error desired in the approximate solution.
c
c       gtol is a nonnegative input variable. termination
c         occurs when the cosine of the angle between fvec and
c         any column of the jacobian is at most gtol in absolute
c         value. therefore, gtol measures the orthogonality
c         desired between the function vector and the columns
c         of the jacobian.
c
c       maxfev is a positive integer input variable. termination
c         occurs when the number of calls to fcn with iflag = 1
c         has reached maxfev.
c
c       diag is an array of length n. if mode = 1 (see
c         below), diag is internally set. if mode = 2, diag
c         must contain positive entries that serve as
c         multiplicative scale factors for the variables.
c
c       mode is an integer input variable. if mode = 1, the
c         variables will be scaled internally. if mode = 2,
c         the scaling is specified by the input diag. other
c         values of mode are equivalent to mode = 1.
c
c       factor is a positive input variable used in determining the
c         initial step bound. this bound is set to the product of
c         factor and the euclidean norm of diag*x if nonzero, or else
c         to factor itself. in most cases factor should lie in the
c         interval (.1,100.).100. is a generally recommended value.
c
c       nprint is an integer input variable that enables controlled
c         printing of iterates if it is positive. in this case,
c         fcn is called with iflag = 0 at the beginning of the first
c         iteration and every nprint iterations thereafter and
c         immediately prior to return, with x, fvec, and fjac
c         available for printing. fvec and fjac should not be
c         altered. if nprint is not positive, no special calls
c         of fcn with iflag = 0 are made.
c
c       info is an integer output variable. if the user has
c         terminated execution, info is set to the (negative)
c         value of iflag. see description of fcn. otherwise,
c         info is set as follows.
c
```

```
c          info = 0  improper input parameters.
c
c          info = 1  both actual and predicted relative reductions
c                    in the sum of squares are at most ftol.
c
c          info = 2  relative error between two consecutive iterates
c                    is at most xtol.
c
c          info = 3  conditions for info = 1 and info = 2 both hold.
c
c          info = 4  the cosine of the angle between fvec and any
c                    column of the jacobian is at most gtol in
c                    absolute value.
c
c          info = 5  number of calls to fcn with iflag = 1 has
c                    reached maxfev.
c
c          info = 6  ftol is too small. no further reduction in
c                    the sum of squares is possible.
c
c          info = 7  xtol is too small. no further improvement in
c                    the approximate solution x is possible.
c
c          info = 8  gtol is too small. fvec is orthogonal to the
c                    columns of the jacobian to machine precision.
c
c        nfev is an integer output variable set to the number of
c          calls to fcn with iflag = 1.
c
c        njev is an integer output variable set to the number of
c          calls to fcn with iflag = 2.
c
c        ipvt is an integer output array of length n. ipvt
c          defines a permutation matrix p such that jac*p = q*r,
c          where jac is the final calculated jacobian, q is
c          orthogonal (not stored), and r is upper triangular
c          with diagonal elements of nonincreasing magnitude.
c          column j of p is column ipvt(j) of the identity matrix.
c
c        qtf is an output array of length n which contains
c          the first n elements of the vector (q transpose)*fvec.
c
c        wa1, wa2, and wa3 are work arrays of length n.
c
c        wa4 is a work array of length m.
c
c      subprograms called
c
c        user supplied ...... fcn
c
c        minpack supplied ... dpmpar,enorm,lmpar,qrfac
c
c        fortran supplied ... dabs,dmax1,dmin1,dsqrt,mod
c
c      argonne national laboratory. minpack project. march 1980.
c      burton s. garbow, kenneth e. hillstrom, jorge j. more
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